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Pauli-Potential and Green Function Monte-Carlo Method for Many-Fermion Systems

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Abstract

The time evolution of a many-fermion system can be described by a Green's function corresponding to an effective potential, which takes anti-symmetrization of the wave function into account, called the Pauli-potential. We show that this idea can be combined with the Green's Function Monte Carlo method to accurately simulate a system of many non-relativistic fermions. The method is illustrated by the example of systems of several (2-9) fermions in a square well.

1 Introduction

The application of Green's Function Monte-Carlo (GFMC) algorithms for the simulation of bosonic and fermionic systems is well known [1], [2]. However, the fermionic case is much more difficult to deal with than the bosonic one [2], [3], [4]. In the framework of simulations of many-fermion systems employing the Langevin equation, Tursunov and Zhirov [5] introduced the idea of a Pauli-potential, to account for the repulsive forces between fermions due to

anti-symmetrization. We study the implementation of this idea in the more efficient GFMC method.

In this work we first describe the standard GFMC method, then we discuss the proposal of Tursunov and Zhirov. After that we illustrate the implementation of the proposed approach within the frame work of GFMC calculations of the simple quantum mechanical system of several fermions in a square well. With moderate computational effort we simulate nine spinless fermions

2 The Green's Function Monte Carlo Algorithm

In the paper [5] the authors applied the Langevin-equation to study multi-fermion systems. We use a more efficient method: Green's Function Monte Carlo [1], [2] in a modified form [6]. The idea of the GFMC-method is to determine the ground-state energy and wave function by operating iteratively with the Green's function on an arbitrary function. The Green's function itself is obtained as a solution of the standard resolvent integral equation:

$$G(E) = G_T(E) + G(E)\,(V - V_T)\,G_T(E). \tag{1}$$

The (exactly known) Green's function $G_T(E)$ is the resolvent for the Hamiltonian with the potential V_T. The time evolution of the system is determined by the propagator in the time representation. For imaginary time this propagator is the Laplace-transform of $G(E)$. Because we solve eq. (1) by iteration using the standard MC method, in order to achieve fast convergence, it is important to employ a trial potential V_T that is as close as possible to V. Besides this trial potential, there are other elements in the GFMC-method that make that method so efficient compared to other stochastic methods. These features are: the guidance function Ψ_G that guides the MC process and the trial energy E_T; the details of the standard GFMC-method are described in the Appendix.

We use the modified algorithm proposed in ref.[6]; which allows to work with the integral equation of the type (1) even in the case where the kernel is not positive definite. In the standard approach the wave-function is represented by a set of points, which move randomly and may disappear

or reappear with some multiplicity, proportional to the kernel of the integral equation (see step 8 of the algorithm described in the Appendix). In the modified GFMC method the multiplicity m_I (see (A.8)) is proportional to the absolute value of the kernel, and all points which are going to the intermediate generation with that multiplicity, also change their phase: $\delta(x) \rightarrow \delta(x) + \delta_K$, where δ_K is the phase of the kernel K which enters into the definition of m_I (A.8). To explain this modification we give a simple example. To calculate the "expectation value" $< \phi >= \int \phi(x) f(x)\, dx / \int f(x)\, dx$ for the complex function $f(x)$ we can generate the set of points $\{x_k\}$ with the probability proportional to $|f(x)|$, and calculate $< \phi >= \sum_k \phi(x_k) e^{i\delta_k} / \sum_k e^{i\delta_k}$ where δ_k is the phase of $f(x_k)$. Of course, the convergence of this procedure is not guaranteed for all choices of ϕ and f. Our results show that for the case studied here (fermions in a square well) there exists a sufficiently broad range of parameters of the algorithm, in which convergence is obtained.

The simple improvement described above allows for inclusion of the sign of the wave function: the density of points corresponds to the magnitude of the wave function. The phase of a point corresponds to the phase of the wave function at that particular position. In this way we are also able to accommodate dynamical nodes in the wave function, which occur in fermionic systems already in the ground state. Our algorithm provides the dynamical nodes in the wave function owing to the action of the Pauli-potential V^F (7).

3 The Idea of Tursunov and Zhirov

The main complication for the use of stochastic simulations of multi-fermion systems is the fact that its wave function must be anti-symmetrized. A basic tool of the methods used here is the imaginary-time single-particle propagator

$$U\left(\mathbf{x}^f, \mathbf{x}^{in}; \beta\right) = C \exp\left\{ -\frac{m\left(\mathbf{x}^f - \mathbf{x}^{in}\right)^2}{2\beta} - \beta V\left(\frac{\mathbf{x}^f + \mathbf{x}^{in}}{2}\right)\right\}, \qquad (2)$$

where m is the mass of the particle and β is a (small) time step. For two identical fermions, 1,2, the imaginary-time propagator can be written as:

$$U^{(F)}\left(\mathbf{x}_1^f, \mathbf{x}_2^f, \mathbf{x}_1^{in}, \mathbf{x}_2^{in}; \beta\right) \;\; =$$

$$U^{(D)}\left(\mathbf{x}_1^f, \mathbf{x}_2^f, \mathbf{x}_1^{in}, \mathbf{x}_2^{in}; \beta\right) \quad - \quad U^{(D)}\left(\mathbf{x}_2^f, \mathbf{x}_1^f, \mathbf{x}_1^{in}, \mathbf{x}_2^{in}; \beta\right), \tag{3}$$

where (F) refers to fermions and (D) to distinguishable particles. $U^{(D)}$ is the product of two single-particle propagators:

$$U^{(D)}\left(\mathbf{x}_1^f, \mathbf{x}_2^f, \mathbf{x}_1^{in}, \mathbf{x}_2^{in}; \beta\right) = U\left(\mathbf{x}_1^f, \mathbf{x}_1^{in}; \beta\right) U\left(\mathbf{x}_2^f, \mathbf{x}_2^{in}; \beta\right) \tag{4}$$

At small values of β, anti-symmetrization (3) can be effectively implemented [5] by using an additional effective potential:

$$\begin{aligned} U^F(1,2) &= U^D(1,2) - U^D(2,1) = U^D(1,2)\left(1 - U^D(2,1)/U^D(1,2)\right) \\ &\approx U^D(1,2) e^{-\beta V^F(1,2)}. \end{aligned} \tag{5}$$

This additional potential, $V^{(F)}$, has the following form to leading order in β:

$$V^{(F)}(1,2) = -\frac{1}{\beta} \ln\left[1 - \exp\left(-\frac{m(\mathbf{x}_1^f - \mathbf{x}_2^f)\cdot(\mathbf{x}_1^{in} - \mathbf{x}_2^{in})}{\beta}\right)\right]. \tag{6}$$

We see that the Pauli-exclusion principle leads to a complex, nonlocal and time-dependent potential; still, it can be used in the Monte-Carlo algorithm.

For the N-fermion case we will have

$$\begin{aligned} V^{(F)}(1,\ldots,N) = & \\ & \tfrac{-1}{\beta} \ln\left[1 - \exp\left(-\textstyle\sum_{k<l} \frac{m(x_k^f - x_l^f)\cdot(x_k^{in} - x_l^{in})}{\beta}\right)\right]. \end{aligned} \tag{7}$$

So, to leading order in β, this "Pauli-potential" corresponds to anti-symmetrization of pairs of particles only: the sum in eq. (7) has only N(N-1)/2 terms. It is very important that the permutations of three and more particles occur when the time-development of the system is simulated by repeated operation of the propagator $U^{(F)}$, *i.e.*, by the repeated action of the potential V^F [5] during the Monte Carlo procedure.

4 Results

We obtained our results by solving eq. (1) in the time-representation. Using this Green's function, we obtain the ground-state wave function of the system

dependent on time: $\psi_0(x;\beta) \sim \exp(-E_0\beta)\psi_0(x;0)$. For an N-particle system in three dimensions, the wave function is represented in the MC-method by a set of points in 3N–dimensional space. The density of the points in such a population follows modulus of the wave function $|\psi_0(x;\beta)|$. The action of the density matrix (Laplace-transformed Green's function) is performed in finite imaginary time steps β.

In order to obtain the Green's function, we perform a Laplace transform of the density matrix by sampling β from the distribution $\exp(-\beta/\Delta)/\Delta$. We varied Δ in order to be able to extrapolate our results to the point $\Delta = 0$, which means that, on average, the time step β tends to zero, since we used the Pauli-potential only to leading order in β.

In order to determine the energy E_0 of the ground state, we monitor the size of the population in time and use (A.13) from the Appendix.

We found that we could decrease the fluctuations in the energy by an order of magnitude if we would kill all points that have a multiplicity (see items 4 and 5 of the GFMC algorithm described in the Appendix) larger than some value M_{max} (Typically $M_{max} \approx 5 - 20$). By this procedure we introduce a systematic error proportional to Δ. Doing so, we do not change the character of the systematic error: it remains linear in Δ.

For a check of our approach we have, until now, studied the case of several spinless fermions in a square-well potential. The number of particles in this well was varied between two and nine.

For the trial potential V_T we use the oscillator interaction, for which the Green's function is known in closed form (A.6) [7]. For the guidance function ψ_G we use a Slater determinant of harmonic-oscillator wave functions. (These may or may not correspond to the same oscillator as is used for the trial potential.)

In Fig.1 we show for a value of $\Delta = 0.0005$ the development of the energy for a system of nine fermions with the number of time steps. In this calculation we use a square well with depth $V_0 = -3.5$, radius $R = 2$; the number of points in each population (which describes the nine fermion wave function) was approximately one thousand. Clearly, the energy converges to a value of -12.8, which differs from the true value (-11.501), indicated by the broken line. The reason for this phenomenon is the fact that we still have a finite Δ.

In order to see the effect of taking smaller time steps, we calculated the energy for different values of Δ. Fig.2 shows this dependence of the average

energy for the same problem on the size of Δ. We clearly see that the average energy tends to the exact energy if Δ tends to zero. Extrapolation of the energy values to the point $\Delta = 0$ gives a value that is almost equal, within the error bars to the exact value for this case (-11.501). These simulations were performed for a value of $E_T = -10.5$, differing from the exact value of the energy, to mimic a realistic situation, when the value of the exact energy is not known.

The true value of the energy can be found by extrapolating the computed values to $\Delta = 0$. We illustrate this for the case of nine bodies in Fig. 3. The number of killed points (taking into account their multiplicities) divided by the total number of points in our simulation process is plotted as a function of Δ. We see that this number indeed depends linearly on Δ. A value $M_{max} = 5$ was taken. We checked that a similar linear dependence occurs when we change M_{max}.

The dependence of the average energy on Δ is shown in Fig. 4 for the case of five fermions in the same square-well potential. The linear dependence of the energy on Δ is clearly seen to occur for sufficiently small values of Δ.

We also found that the Pauli potential acts in such a way that the motion of points that render the argument of the logarithm in eqs. (6,7) negative, is hindered. We checked, by recording the number of points that do cross the border, that the Pauli repulsion effectively blocks the crossing, for $\Delta\beta \to 0$.

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Appendix A

Below we describe the main steps of the algorithm [2] (see also the pedagogical paper [8] or the book by Kalos and Whitlock [9]) for the solution of the integral equation (1).

1. A set of points is sampled from a distribution $f_1(x) = |\Psi_G(x)|^2$. For N fermions in D dimensions x is a DN-dimensional vector representing the positions of N particles (if we exclude the center of mass motion it is an $(N-1)D$-dimensional vector). For the initial distribution we take $|\Psi_G(x)|^2$, because eventually we will obtain from the process the distribution $\Psi(x)\Psi_G(x)$ rather than $\Psi(x)$. The typical number of points in this set, called the initial generation, is several hundreds.

2. It is convenient to work with the density matrix $\rho(x, x', \beta) = \sum_n \Psi_n^*(x)\Psi_n(x')e^{-E_n\beta}$. The density matrix is related to the Green's function $G(x, x', E)$ by the Laplace transform. In our algorithm we carried out the Laplace transform by sampling the imaginary time β from the distribution $\frac{1}{\Delta}\exp\left\{-\frac{\beta}{\Delta}\right\}$. found that the additional random number occurring in the sampling of the imaginary-time distribution involved in the Laplace transform, improves the statistical errors.

3. To each point x' in the initial generation the diffusion and drift is applied, after which the points are distributed with the probability

$$f(x, \beta) = \int \rho_D(x, x', \beta) f_1(x')\, dx', \tag{A.1}$$

where

$$\rho_D(x, x', \beta) = \left(\frac{m}{2\pi\beta}\right)^{\frac{DN}{2}} \exp\left\{-\frac{m(x - x' - \beta F(x'))^2}{2\beta}\right\} \tag{A.2}$$

m is the mass of the fermion and the "quantum force" F is given by:

$$F_i(x) = \frac{1}{m}\Psi_G^{-1}(x)\frac{\partial}{\partial x_i}\Psi_G(x), \tag{A.3}$$

Note that $F_i(x)$ is the component of a vector as $\frac{\partial}{\partial x_i}$ is.

Because ρ_D does not enter the final expression, as the dependence on ρ_D is cancelled due to the fact that ρ_D enters also in the denominator of m_D (see (A.4)) the random walk of points can be performed with an arbitrary probability distribution. For the distance probability distribution a Gaussian form is used, since random numbers with a Gaussian distribution can be generated very efficiently on a computer. The second reason for choosing this distribution is, that it is similar to the real distribution corresponding to the bound state.

Algorithmically the sampling of the distribution (A.1) is done in two steps. First we shift the initial points: $x'' = x' + \beta F(x')$, and after that we add to each point the gaussian random numbers η_i with unit expectation value: $x_i = x''_i + \sqrt{\frac{2\beta}{m}}\eta_i$

4. In order to construct the new generation, multiple copies of each point x are produced. The multiplicity is given by the formula:

$$m_D(x, x', \beta) = e^{E_T\beta} \frac{\Psi_G(x)}{\Psi_G(x')} \frac{\rho_T(x, x', \beta)}{\rho_D(x, x', \beta)} \tag{A.4}$$

where ρ_T is the density matrix (the Laplace-transformed Green's function) for the trial potential which satisfies the well known equation:

$$\frac{\partial \rho_T(x, x', \beta)}{\partial \beta} = -H_T \rho(x, x', \beta);\ \rho_T(x, x', 0) = \delta(x - x'). \tag{A.5}$$

For the trial hamiltonian we use the harmonic oscillator hamiltonian, for which ρ_T is known explicitly [7]:

$$\begin{aligned} \rho_T(x, x', \beta) &= \left(\frac{m\omega_T}{2\pi \sinh \omega_T\beta}\right)^{\frac{ND}{2}} \\ &\times \exp\left\{-\frac{m\omega_T}{2\sinh\omega_T\beta}[(x^2 + x'^2)\cosh\omega_T\beta - 2x \cdot x'] - c_T\beta\right\} \end{aligned} \tag{A.6}$$

This trial density matrix corresponds to a hamiltonian with the potential V_T, given by

$$V_T(x) = \frac{m\omega_T^2 x^2}{2} + c_T. \tag{A.7}$$

The trial energy E_T is introduced in order to avoid exponential growth or shrinkage of the number of points of the population. As a result, the number of points in the population fluctuates around a value that has the time-dependence $\exp\{-(E_0 - E_T)\beta\}$. Effectively, this amounts to a shift in the hamiltonian with the constant energy E_T.

5. The other, so called intermediate, branch of the process is formed by creating another set of multiple copies of the points x: for them the multiplicity is given by:

$$m_I(x, x', \beta) = \frac{K(x, x', \beta) m_D(x, x', \beta)\Delta}{\rho_T(x, x', \beta)}, \tag{A.8}$$

here K is the Laplace transformed kernel of the integral equation (1),

$$K(x, x', \beta) = [V_T(x) - V(x)]\rho_T(x, x', \beta). \tag{A.9}$$

In general m_D and m_I are not integers. We convert them to integers by adding a uniformly distributed random number to each of them and take the integer part.

6. Each intermediate point, created this way, is treated in the same way as the points taken from the initial generation, *i.e.*, they will take part in the random walk with branching until they are eventually propagated to the new generation. If the average value of m_I is less than unity, this process is completed in a finite time on the computer.

The sequence of operations described above, correspond to the terms in the iterative solution of the equation:

$$\tilde{\rho} = \tilde{\rho}_T + \Delta \cdot K * \tilde{\rho} \tag{A.10}$$

where $K = V$ and $*$ denotes the integration over the intermediate coordinates: $K * \tilde{\rho} = \int K(x, x'')\tilde{\rho}(x'', x')\, dx''$. The direct points correspond to the term $\tilde{\rho}_T$, while the intermediate points correspond to $\Delta \cdot K$. If an intermediate point is processed again, it may be promoted immediately to the new

generation, in which case it corresponds to the term $\Delta \cdot \tilde{\rho}_T * K$, otherwise it will be an intermediate point again, now corresponding to $\Delta^2 \cdot K * K$ etc. The difference in the normalization of the kernels of the equations (1) and (A.10) is due to the difference in the normalization of G and $\tilde{\rho}$:

$$\begin{aligned} \tilde{\rho}(x,x') &= \frac{1}{\Delta}\frac{\Psi_G(x)}{\Psi_G(x')}G(x,x',E_T-\frac{1}{\Delta}) \\ &= \frac{\Psi_G(x)}{\Psi_G(x')}\sum_n \frac{\Psi_n^*(x)\Psi_n(x')}{1+\Delta(E_n-E_T)} \end{aligned} \tag{A.11}$$

here $\Psi_n(x)$ and E_n are the wave function and the energy of the n-th level of the Hamiltonian studied here. The distribution of points in the new (second) generation is sampled with the probability distribution

$$f_2(x) = \int \tilde{\rho}(x,x') f_1(x')\, dx'. \tag{A.12}$$

In the same way we can get the distributions $f_3, ..., f_n$;

Using expression (A.11) for $\tilde{\rho}(x,x')$ it is easy to prove that as $n \to \infty$ $f_n(x) \to const.\Psi_G(x)\Psi_0(x)/[1+\Delta(E_0-E_T)]^{n-1} + ...$, where $\Psi_0(x)$ and E_0 are the wave function and the energy of the ground state. So the ground state energy can be calculated from the number of points, P_n in the n-th generation:

$$E_0 = E_T + \frac{1}{\Delta}\left(\frac{P_{n-1}}{P_n} - 1\right). \tag{A.13}$$

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Figure Captions

Fig. 1 The development with the number of time steps (N) of the energy for a system of nine fermions. The value of Δ is 0.0005.

Fig. 2 Dependence of the energy of the system of nine fermions on the time step Δ. A linear fit is made, which gives an estimate of the energy for $\Delta = 0$.

Fig. 3 The dependence on Δ of the number of killed points for the system of nine fermions divided by the total number of points in our simulation. The parameter $M_{max} = 5$.

Fig. 4 The same as Fig. 2, but now for five fermions. It is seen that the linear dependence of the energy on Δ obtains for small values of Δ. A linear fit of the points at low values of Δ intersects the axis at the exact energy (indicated by the broken line).

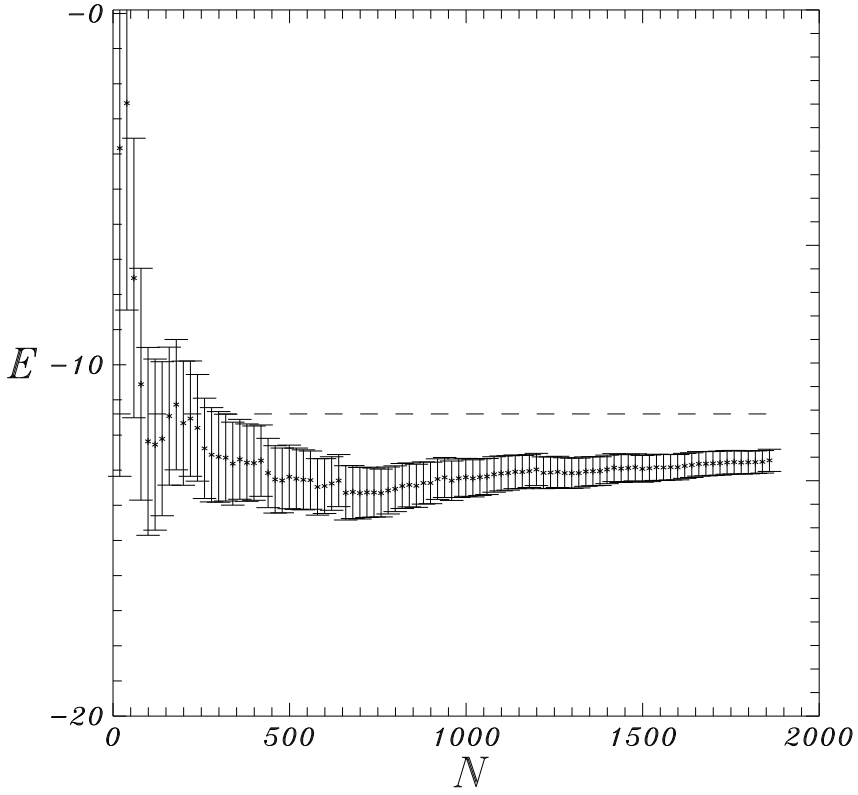


Fig. 1

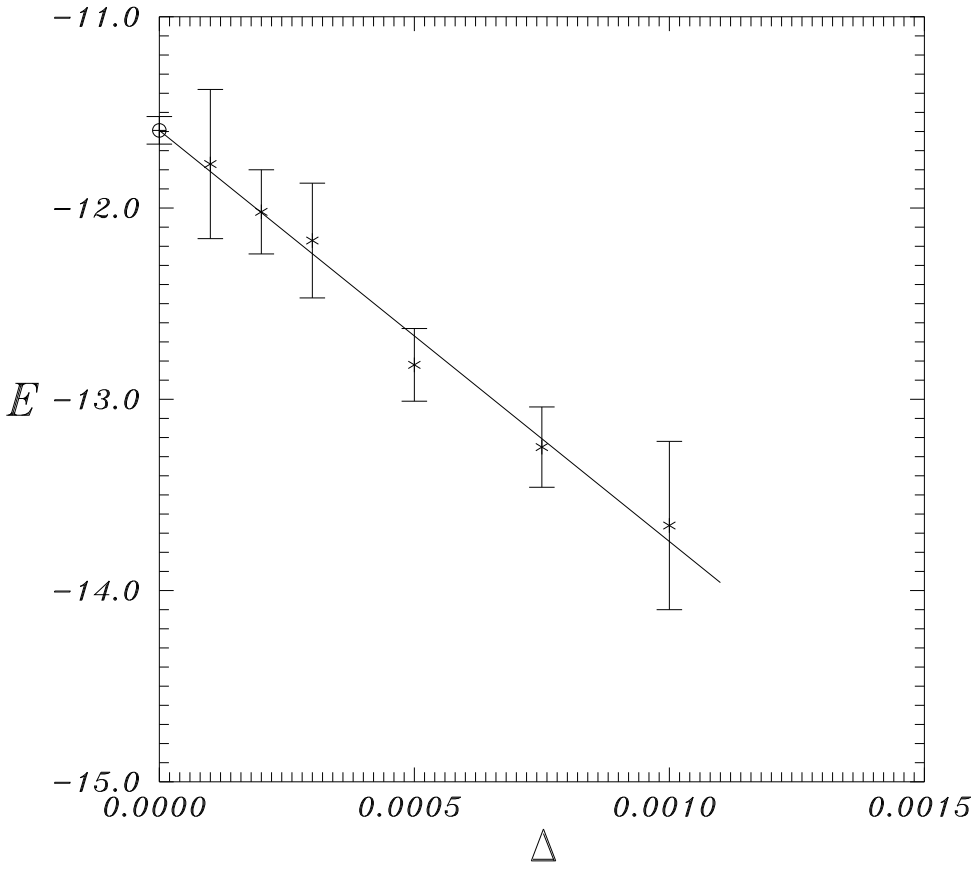
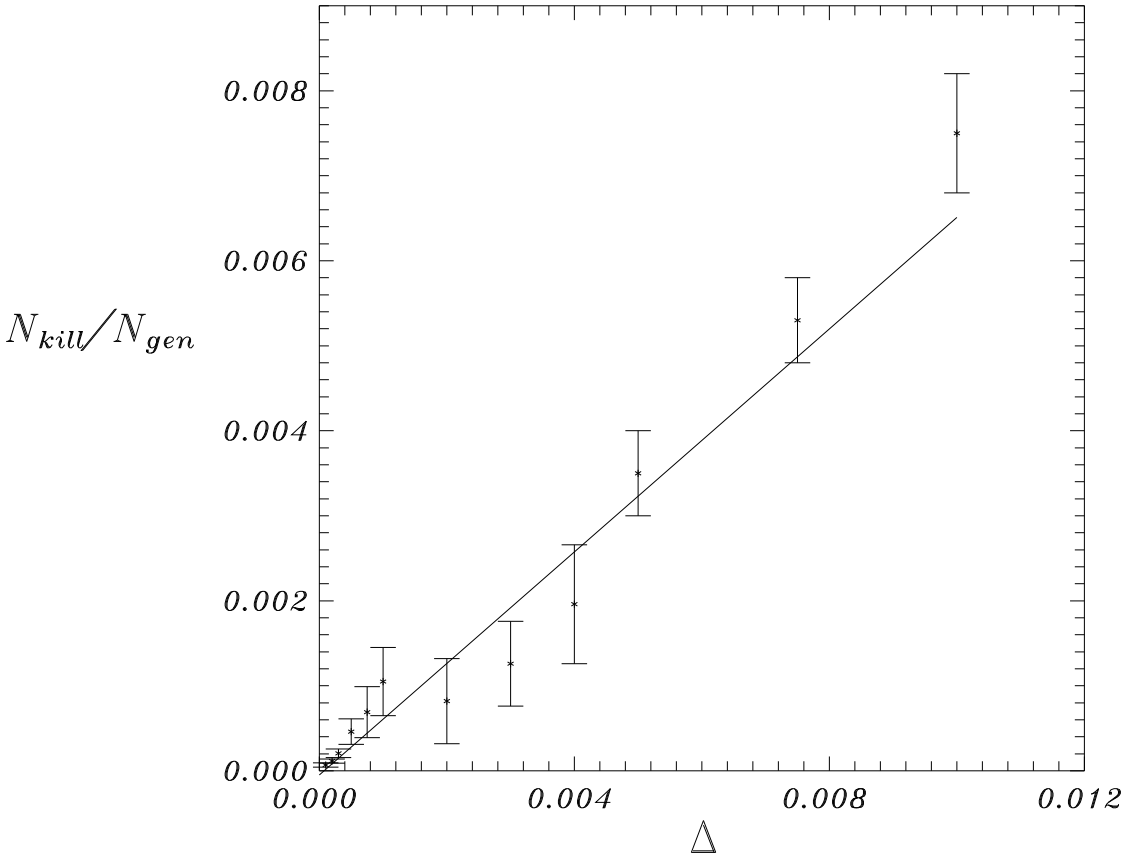


Fig. 2


0.008
0.006
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0.000
N_{kill}/N_{gen}
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0.008
0.012
Δ

Fig. 3

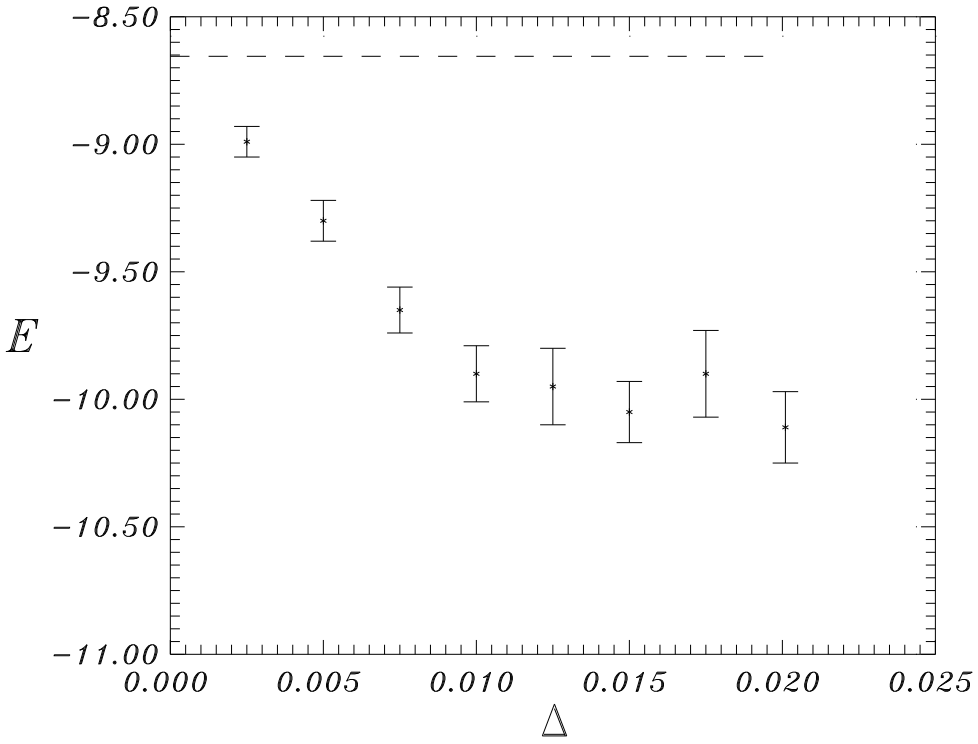

Fig. 4